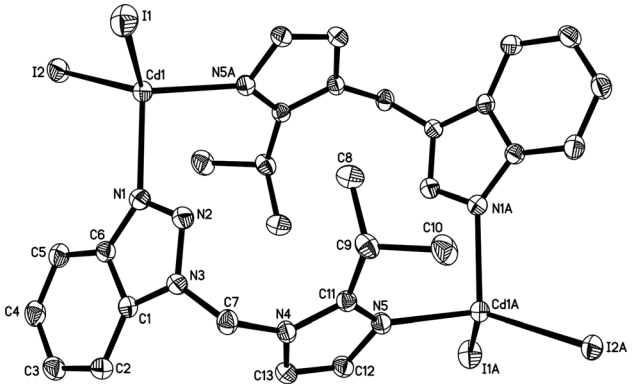
Hai-Yan Yang*, Hong-Fang Wang, Hui Li, Ying-Hua Li and Yao-Min Zhao

Crystal structure of *cyclo*[tetraiodido-bis{μ_2-1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-isopropyl-imidazol)-k^2*N:N*}dicadmiun(II)], $C_{26}H_{30}N_{10}Cd_2I_4$



https://doi.org/10.1515/ncrs-2023-0209
Received April 28, 2023; accepted July 4, 2023;
published online July 25, 2023

Abstract

$C_{26}H_{30}N_{10}I_4Cd_2$, monoclinic, $P2_1/n$ (no. 14), a = 8.1164(10) Å, b = 15.9401(18) Å, c = 13.5531(17) Å, β = 96.067(4)°, V = 1743.6(4) Å^3, Z = 2, $R_{gt}(F)$ = 0.0394, $\omega R_{ref}(F^2)$ = 0.1088, T = 273 K.

CCDC no.: 2279143

Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

1 Source of material

A methanol solution (4 mL) of 1-((benzotriazol-1-yl)methyl)-1-*H*-1,3-(2-isopropyl-imidazol) (0.05 mmol) was added dropwise into a methanol solution (4 mL) of CdI_2 (0.05 mmol), giving a clear solution. The resulting solution was left at room temperature. After five days, good quality colorless crystals were obtained from the solution.

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	0.15 × 0.14 × 0.12 mm
Wavelength:	Mo *K*α radiation (0.71073 Å)
μ:	4.79 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω
θ_{max}, completeness:	27.5°, 99 %
$N(hkl)_{measured}$, $N(hkl)_{unique}$, R_{int}:	47,046, 3976, 0.152
Criterion for I_{obs}, $N(hkl)_{gt}$:	$I_{obs} > 2\sigma(I_{obs})$, 3773
$N(param)_{refined}$:	192
Programs:	CrysAlis^{PRO} [1], Olex2 [2], SHELX [3]

2 Experimental details

H atoms were generated geometrically, with C–H = 0.96, 0.97 and 0.93 Å for methyl, methylene and aromatic H, respectively, and constrained to ride on their parent atoms with U_{iso}(H) = x times U_{eq}(C), where x = 1.5 for methyl H and x = 1.2 for all other H atoms.

3 Comment

Coordination compounds have attracted interest because of their interesting structures, topologies, properties and their potential applications as functional materials [4, 5]. Multidentate N-heterocyclic ligands containing rich coordination sites, such as imidazole, triazole, tetrazole and their derivative are often employed to produce polymeric networks with structural diversity [6, 7]. And for some time we have involved in the synthesis of a series of multidentate N-heterocyclic compounds and studied their coordination behaviors [8–10]. Recently, our group synthesized a compound based on the imidazol and benzotriazol, 1-[(benzotriazol-1-yl) methyl]-1-*H*-1,3-(2-methyl-imidazol), and studied its coordination behavior [11–14]. As a continuation of our research, we synthesized a compound 1-[(benzotriazol-1-yl)methyl]-1-*H*-1,3-(2-isopropyl-imdazol)(bmipi), and used it as ligand to react with CdI_2, generating a new coordination compound, which is reported here.

***Corresponding author: Hai-Yan Yang**, School of Materials and Chemical Engineering, Zhongyuan University of Technology, Zhengzhou, 450007, P.R. China, E-mail: yanghy0204@163.com. https://orcid.org/0000-0002-7317-0786

Hong-Fang Wang, Hui Li, Ying-Hua Li and Yao-Min Zhao, School of Materials and Chemical Engineering, Zhongyuan University of Technology, Zhengzhou, 450007, P.R. China

Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2).

Atom	*x*	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.62188 (3)	0.75888 (2)	0.47243 (2)	0.03431 (11)
I1	0.34536 (4)	0.83863 (2)	0.39119 (3)	0.05465 (13)
I2	0.89256 (3)	0.85713 (2)	0.51801 (2)	0.04698 (12)
N1	0.6775 (4)	0.6613 (2)	0.3539 (3)	0.0366 (7)
N2	0.5535 (4)	0.6114 (2)	0.3274 (3)	0.0371 (7)
N3	0.6010 (4)	0.55767 (19)	0.2596 (2)	0.0323 (6)
N4	0.5079 (4)	0.4194 (2)	0.2964 (2)	0.0316 (6)
N5	0.4641 (4)	0.33045 (19)	0.4143 (2)	0.0329 (6)
C1	0.7606 (5)	0.5736 (2)	0.2402 (3)	0.0320 (7)
C2	0.8635 (5)	0.5387 (3)	0.1751 (3)	0.0398 (8)
H2	0.829977	0.494305	0.133198	0.048*
C3	1.0180 (5)	0.5745 (3)	0.1771 (4)	0.0448 (9)
H3	1.090599	0.554264	0.133984	0.054*
C4	1.0702 (5)	0.6402 (3)	0.2416 (4)	0.0437 (9)
H4	1.177449	0.660775	0.241584	0.052*
C5	0.9680 (5)	0.6752 (3)	0.3050 (3)	0.0411 (9)
H5	1.002400	0.719185	0.347321	0.049*
C6	0.8093 (5)	0.6407 (2)	0.3022 (3)	0.0329 (7)
C7	0.4918 (5)	0.4888 (2)	0.2262 (3)	0.0350 (7)
H7A	0.378006	0.508364	0.218645	0.042*
H7B	0.518641	0.469428	0.161954	0.042*
C8	0.2619 (6)	0.5082 (3)	0.4531 (4)	0.0513 (11)
H8A	0.293720	0.483132	0.516661	0.077*
H8B	0.159139	0.537724	0.454908	0.077*
H8C	0.346224	0.546781	0.437534	0.077*
C9	0.2405 (5)	0.4398 (3)	0.3739 (3)	0.0378 (8)
H9	0.205224	0.467517	0.310628	0.045*
C10	0.1022 (5)	0.3792 (3)	0.3949 (4)	0.0532 (11)
H10A	0.100002	0.332697	0.349770	0.080*
H10B	−0.002388	0.407835	0.386322	0.080*
H10C	0.122191	0.358990	0.461847	0.080*
C11	0.4014 (4)	0.3954 (2)	0.3621 (3)	0.0301 (7)
C12	0.6175 (5)	0.3138 (3)	0.3811 (3)	0.0368 (8)
H12	0.690021	0.271678	0.405409	0.044*
C13	0.6447 (5)	0.3678 (2)	0.3088 (3)	0.0375 (8)
H13	0.737357	0.370022	0.273973	0.045*

The title compound is a cyclic, dinuclear structure. As is shown in the Figure, the Cd (II) atom is four-coordinated by two N atoms from two bmipi ligands, with Cd–N bond lengths of 2.315(3) Å and 2.258(3) Å, and two I atoms, with Cd–I bond lengths of 2.7098(5) Å and 2.7156(4) Å. The bond angles around the Cd atom vary from 98.34(12)° (N5A–Cd1–N1) to 120.64(9)° (N5A–Cd1–I2). In the crystal, the adjacent molecules are stacked through intermolecular interactions to form a supramolecular compound [15].

Author contributions: All the authors have accepted responsibility for the entire content of this submitted manuscript and approved submission.

Research funding: The authors are grateful to Zhongyuan University of Technology.

Conflict of interest statement: The authors declare no conflicts of interest regarding this article.

References

1. Agilent Technologies. CrysAlis^{PRO} *Software System, Version 171.35.15*; Agilent Technologies UK Ltd: Oxford, UK, 2011.
2. Dolomanov O. V., Bourhis L. J., Gildea R. J., Howard J. A. K., Puschmann H. OLEX2: a complete structure solution, refinement and analysis program. *J. Appl. Crystallogr.* 2009, *42*, 339–341.
3. Sheldrick G. M. A short history of *SHELX*. *Acta Crystallogr.* 2008, *A64*, 112–122.
4. Li H., Eddaoudi M., O'Keeffe M., Yaghi O. M. Design and synthesis of an exceptionally stable and highly porous metal-organic framework. *Nature* 1999, *402*, 276–279.
5. Chesnut D. J., Hagrman D., Zapf P. J., Hammond R. P., Duca R. L., Haushalter R. C., Zubieta J. Organic/inorganic composite materials: the roles of organoamine ligands in the design of inorganic solids. *Coord. Chem. Rev.* 1999, *190–192*, 737–769.
6. Yang Y., Jiang F. L., Liu C. P., Chen L., Gai Y. L., Pang J. D., Su K. Z., Wan X. Y., Hong M. C. Self-assembly syntheses, structural characterization, and luminescent properties of lanthanide coordination polymers constructed by three triazole-carboxylate ligands. *Cryst. Growth Des.* 2016, *16*, 2266–2276.
7. Seth S., Matzger A. J. Coordination polymerization of 5,5′-dinitro-2*H*,2H′-3,3′-bi-1,2,4-triazole leads to a dense explosive with high thermal stability. *Inorg. Chem.* 2017, *56*, 561–565.
8. Yang H.-Y., Li L.-K., Wu J., Hou H.-W., Xiao B., Fan Y.-T. 3D coordination framework with uncommon two-fold interpenetrated $\{3^3{\cdot}5^9{\cdot}6^3\}$-lcy net and coordinated anion exchange. *Chem. Eur. J.* 2009, *15*, 4049–4056.
9. Mu Y.-J., Fu J.-H., Song Y.-J., Li Z., Hou H.-W., Fan Y.-T. Hydrothermal syntheses of metal-organic frameworks constructed from aromatic polycarboxylate and 4,4′-bis(1,2,4-triazol-1-ylmethyl)biphenyl. *Cryst. Growth Des.* 2011, *11*, 2183–2193.
10. Liu L., Huang C., Xue X.-N., Li M., Hou H.-W., Fan Y.-T. Ni(II) Coordination polymers constructed from the flexible tetracarboxylic acid and different N-donor ligands: structural diversity and catalytic activity. *Cryst. Growth Des.* 2015, *15*, 4507–4517.
11. Yang H.-Y., Li Y.-H., Chen H. Crystal structure of bis{1-[(benzotriazol-1-yl)-methyl]-1-*H*-1,3-(2-methyl-imidazol)}-di- iodidocadmium(II), $C_{22}H_{22}CdI_2N_{10}$. *Z. Kristallogr. N. Cryst. Struct.* 2012, *227*, 527–528.
12. Yang H.-Y., Li Y.-H. Crystal structure of bis{1-[(benzotriazol-1-yl)-methyl]-1-*H*-1,3-(2-methyl-imidazol)}-dibromidomercury(II), $C_{22}H_{22}Br_2HgN_{10}$. *Z. Kristallogr. N. Cryst. Struct.* 2014, *229*, 83–84.
13. Yang H.-Y. Crystal structure of aquadichloridobis(1-((2-methyl-1*H*-imidazol-1-yl)methyl)-1*H*-benotriazole-κ*N*)mercury(II), $C_{22}H_{24}HgCl_2N_{10}O$. *Z. Kristallogr. N. Cryst. Struct.* 2016, *231*, 687–688.
14. Yang H.-Y., He F., Zhao Y.-M., Li H., Wang H.-F., Li Y.-H. Crystal structure of bis{1-[(benzotriazol-1-yl)-methyl]-1-*H*-1,3-(2-methyl-imidazol)}-diiodidocadmium(II), $C_{22}H_{22}CdI_2N_{10}$. *Z. Kristallogr. N. Cryst. Struct.* 2019, *233*, 919–921.
15. Wang X., Niu J.-l. Bis{*μ*-1-[(2-ethyl-1*H*-imidazol-1-yl)methyl]-1*H*-benzotriazole}bis(iodidocadmium). *Acta Crystallogr.* 2011, *E67*, m882.